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ON THE STRUCTURE OF LAMINAR DIFFUSION FLAMES

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ABSTRACT

The structure of laminar diffusion flames is analyzed in the limiting case of large, although finite, reaction rates.

It is shown that the chemical reaction takes place only in a very thin region or «chemical boundary layer» where convection effects may be neglected. Then the temperature and mass fraction distributions within the reaction zone are obtained analytically.

The flame position, rates of fuel consumption, and temperature and concentration distributions outside of the reaction zone may be obtained by using the assumption of infinite reaction rates.

For large Reynolds numbers mixing and combustion take place in boundary layers and free mixing layers. And again analytical solutions are obtained for the temperature and mass fraction distributions outside of the reaction zone.

NOMENCLATURE

The following is a list of the most important symbols used in this paper.

A_0 Parameter given by [44], that measures the deviations from the Burke-Schumann solution.

c_p Specific heat at constant pressure.

D   Diffusion coefficient.

E   Activation energy of the chemical reaction.

f Dimensionless stream function.

K_i Mass fraction of species i.

L   Some overall characteristic length.

M   Mean molecular mass.

$\dot{m}$ Mass rate of fuel comsumption per unit flame surface.

Pr   Prandtl number.

p Pressure.

q Heat released per unit mass of fuel.

R   Universal gas constant.

Re   Reynolds number.

Sc   Schmidt number.

T   Temperature.

T_f Adiabatic flame temperature given by [24].

T_c Temperature at the ideal flame surface.

t_c Characteristic chemical time defined by [15].

t_m Characteristic mixing time, $t_m = \delta_m^2/D_0$.

U   Characteristic overall velocity.

u, v Velocity components in boundary layer coordinates.

$\vec{v}$ Velocity vector.

$\vec{v}_{di}$ Diffusion velocity of species i.

w_i Mass production rate, per unit volume, of species i.

X, Y   Mixing boundary layer coordinates.

$\vec{x}$ Position vector.

x, y Chemical boundary layer coordinates.

$y_1 = \int_0^y (\rho/\rho_0) \, dy$.

$z = y_1/\delta_c$.

β Universal function giving the temperature distribution within the reaction zone. Defined by [39].

δ_m Mixing length, $\delta_m = \rho_0 D_0/\dot{m}$.

δ_c Characteristic thickness of the reaction zone given by [41].

η Dimensionless distance normal to the mixing layer.

θ Non-dimensional temperature. $\theta = (T - T_0)/(T_f - T_0)$.

$\theta_a = E/R(T_f - T_0)$.

$\theta_0 = T_0/(T_f - T_0)$.

$\theta_c = (T_c - T_0)/(T_f - T_0)$.

λ u_F/u_0.

μ Viscosity coefficient.

ν Stoichiometric ratio species 2 to 1.

ξ Non-dimensional distance along the mixing layer.

ρ Density.

$\underline{\underline{\sigma}}$ Stress tensor.

SUBSCRIPTS:

1, 2, 3   Indicate fuel, oxidizer and products respectively.

$_F$ Indicates conditions at the fuel exit.

$_0$ Indicates conditions on the oxidizer side of the flame, far from the flame.

$_f$ Indicates conditions at the flame surface for infinite reaction rates.

The asterisk is used for the non-dimensional variables introduced in section II. 6.

I. INTRODUCTION

Diffusion flames are obtained when the reacting species are initially separated. Combustion and mixing takes place simultaneously.

In these flames the reaction zone separates the two reacting species which diffuse, through inert gases and combustion products, from each side towards the flame.

The reacting species burn very rapidly as they reach the reaction zone; thereby the combustion velocity is generally conditioned to the accesibility of the species to the reaction

zone; or in other words, to their facility to diffuse across the inert gases and combustion products.

It seems that we can arrive at a description of some of the most important features of diffusion flames by using the assumption, first introduced by Burke and Schumann (1), of infinitely fast reaction rates. Then the actual zones of combustion become infinitely thin, and the mixing process alone becomes responsible for the rate of burning and for flame location and size.

Burke and Schumann have successfully used their assumption for the calculation of the shape and length of the laminar diffusion flame formed when a fuel jet discharges within a tube. In this tube an air stream moves with the same velocity as the fuel jet. The same assumption has been utilized by Hottel and Hawthorne (2), Wohl, Gazley and Kapp (3), Yagi and Saji (4), and Barr (5), for the prediction of the length of open flames, both laminar and turbulent. Through rudimentary approximations they obtain an expression for the flame length containing an unknown function; this they determine empirically from the results of their experiments. Fay (6) has calculated, by using Burke Schumann assumption, the shape and characteristics of the laminar diffusion flame obtained when a fuel jet discharges into the open atmosphere.

The infinite reaction rate assumption has also been utilized (7), (8) for the study of diffusion flames in boundary layers.

In addition, an extensive literature exists on the application of the assumption to fuel droplet combustion.

The Burke-Schumann assumption eliminates chemical kinetics from the process, simplifying the governing equations and their solution. However, this solution does not provide the criterion for the extinction of the flame, or for the validity of the assumption and solution.

Zeldovich (9) has taken into consideration the finite thickness of the reaction zone to explain the blowing-off phenomenon. Similar studies have been performed by Spalding (10), (11), (12) with the purpose of relating the fuel consumption rate per unit area at extinction and the fuel consumption rate per unit area in a premixed flame.

For a general description of the diffusion flames see, for example, the review papers by Barr (13) and Wohl and Shipmann (14), where data and bibliography on the subject can be found.

We aim in this work to show the effects of finite chemical reaction rates on the structure of laminar diffusion flames. In order to do so, we will study certain limiting cases, in which simple analytical solutions can be obtained. We will limit ourselves to the study of one step chemical reactions in which the forward reaction is dominant.

We shall show that for large reaction rates the chemical reaction takes place only in a very thin region or «chemical boundary layer». This has already been shown (15) in the simple case of the mixing and combustion of two parallel streams of fuel and oxidizer moving with the same velocity. There convection effects may be neglected compared with the much more important diffusion conduction and chemical reaction effects. The governing equations reduce in this case to ordinary differential equations. The kinetics of the reaction appears in the solution; but the temperatures are close to the adiabatic flame temperature, and in this range of temperatures the concept of an overall kinetic scheme has been found by Levy and Weinberg (16) to be valid.

The solution with the assumption of infinite reaction rates (which we shall call the Burke-

Schumann solution) represents the true solution outside of the reaction zone. It may also be used to calculate the flame position and fuel consumption per unit flame area.

If the Reynolds number, based on some overall characteristic length, is large, mixing and combustion will take place only in a very thin region or mixing layer, where boundary layer approximations may be used (17), (18), (19).
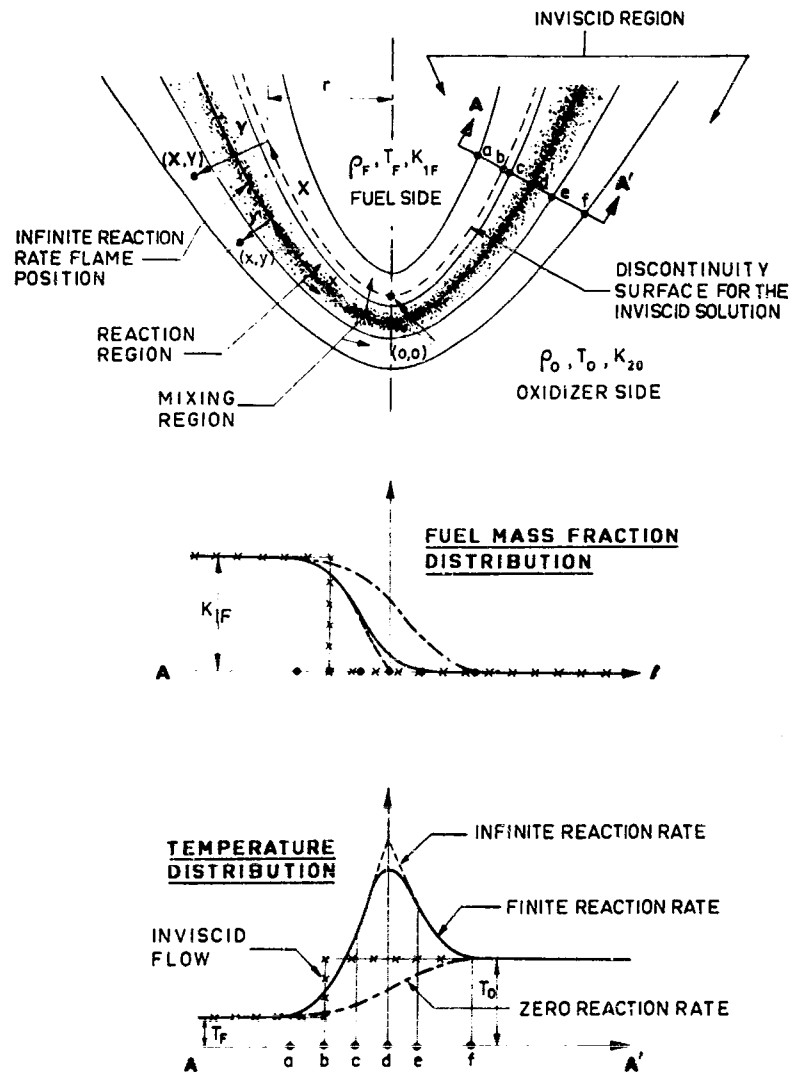

Fig. 1.—Diffusion Flame Structure

The mixing layer location and general flow characteristics outside of the mixing layer may be determined by using the inviscid flow equations. However, we must allow for the existence of discontinuities in the velocity, density, temperature, and mass fraction distributions within the flow field.

In Figure 1 the temperature and mass fraction distributions, as obtained by different limiting assumptions, are schematically represented.

II. General Equations

We shall begin by writing the general equations governing the steady laminar flow of a reacting gas mixture (20), (21), (22). We will use the assumption that the fluid may be considered as a continuous medium formed by a mixture of perfect gases.

Only three species will be considered: Fuel, oxidizer, and products. For the sake of simplicity, any inert species present will be considered as products.

Besides the usual dependent variables of ordinary fluid mechanics, i. e. velocity $\vec{v}$, pressure p, density ρ, and temperature T, three new variables, the mass fractions of the reactant species, enter. Therefore, three new equations, stating the mass conservation law for each of the species, must be added to the fundamental equations of fluid mechanics. In addition, the relations between the transport parameters and mass fractions, temperature, and pressure of the mixture will be required.

We shall use subscript 1 for fuel, 2 for oxidizer, and 3 for the products. The mass fractions of species i will be written

$$K_i \quad \rho_i/\rho.$$

The three mass fractions obviously satisfy the relation

$$K_1 + K_2 + K_3 = 1. \tag{1}$$

II.1. *Equation of State.*

If the fluid is considered as a mixture of perfect gases the equation of state is as follows

$$p = \rho (R/M) T \tag{2}$$

where R is the universal constant of the gases, and

$$M = \left[\sum_1^3 K_i M_i \right]^{-1} \tag{3}$$

is the mean molecular mass.

In order to simplify the calculations we will use a mean constant value for M. This approximation is justified when the molecular masses of the species are not very different or when the reactants are very dilute. Then $M \sim M_3$.

In any case the results will not be essentially changed by considering M as variable.

II.2. *Equation of Continuity for the Mixture.*

This simply states the law of mass conservation

$$\nabla \cdot (\rho \vec{v}) = 0. \tag{4}$$

II.3. *Equations of Mass Conservation for the Species.*

These state that the mass quantity of each constituent entering unit volume per unit time, either due to convection or diffusion, equals the mass quantity of the constituent disappearing as a consequence of the chemical reaction.

These equations are as follows

$$\rho \vec{v} \cdot \nabla K_i + \nabla \cdot (\rho K_i \vec{r}_{di}) = w_i \tag{5}$$

where $\vec{r}_{di}$ is the diffusion velocity of species i, and w_i is the mass production rate per unit volume of species i.

We consider a one step chemical reaction in which the forward reaction is dominant, the backward reaction being negligible. For an Arrhenius type reaction with second order chemical kinetics, we may write

$$w_1/\rho = -b(p/RT)\exp[-E/RT]\cdot K_1 K_2 \tag{6a}$$

where E is the activation energy of the reaction and b is the frequency factor. Also if ν is the stoichiometric ratio oxidizer-fuel

$$w_2 = \nu w_1, \qquad w_3 = -(1+\nu)w_1. \tag{6b}$$

We shall use relation [6a] through most of this study. The extension to more general reaction rates of the form

$$w_1/\rho = -g(T, p)\exp[-E/RT]\cdot K_1^a K_2^b \tag{7}$$

is easily made.

The diffusion velocities depend on pressure, temperature and species concentration gradients. Usually the pressure gradient effect on diffusion velocities is small compared to those due to mass fraction gradients. This is specially true when mixing takes place in thin mixing regions and boundary layers. Thermal diffusion will be neglected because diffusion velocities due to gradients of temperature are generally a small fraction of the velocities due to concentration gradients.

If the molecular masses of the species are approximately equal we may use Fick's law for the determination of $\vec{r}_{di}$.

$$K_i \vec{r}_{di} = -D \nabla K_i \tag{8}$$

where D is an average diffusion coefficient.

If the concentration of one of the species is small, Fick's law is valid for the other two species. This always happens in diffusion flames where oxidizer concentration, for example,

is very small in the reaction zone, or in the fluid side of the flame. Then we may use Fick's law for fuel and oxidizer with the diffusion coefficients determined by the binary mixtures: fuel-products and oxidizer-products respectively. In this study we will use a single average diffusion coefficient D.

Inserting [8] into [5] we obtain

$$\vec{r} \cdot \nabla K_i = (1/\rho) \nabla \cdot (\rho D \nabla K_i) + w_i/\rho. \tag{9}$$

II.4. *Momentum equation.*

$$\vec{v} \cdot \nabla \vec{v} = -(1/\rho) \nabla p + (1/\rho) \nabla \cdot \underline{\sigma}. \tag{10}$$

Where $\underline{\sigma}$ is the stress tensor

$$\sigma_{ij} = -\frac{2}{3} \mu \frac{\partial r_k}{\partial x_k} \delta_{ij} + \mu \left(\frac{\partial r_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right).$$

We neglect the diffusion stress tensor. Gravity forces will also be neglected for simplicity, although they can only be neglected for large Froude numbers and this is not always the case in diffusion flames.

II.5. *Energy Equation.*

If the specific heats c_{p_i} of the species are assumed to be equal and constant the energy equation may be written

$$\vec{r} \cdot \nabla T = \frac{1}{\rho} \nabla \cdot \left(\frac{\mu}{Pr} \nabla T \right) + \frac{1}{\rho c_p} \sigma : \nabla \vec{r} + \frac{1}{\rho c_p} \vec{v} \cdot \nabla p - \frac{w_1}{\rho} \frac{q}{c_p} \tag{11}$$

where $\sigma : \nabla \vec{r}$ is the Rayleigh dissipation function and q is the chemical energy that a combustible mixture containing a unit mass of fuel and ν units of oxidizer has available for conversion into thermal energy $q = h_1^0 + \nu h_2^0 - (1 + \nu) h_3^0$. Pr is the Prandtl number which will be assumed constant. Thermal radiation is not taken into account.

Equations [2], [4], [10], [11] and [9] (for $i = 1, 2$), together with relations [6] and the functional relations between the transport parameters and p, T, and K_i, constitute the system of differential equations governing the structure of diffusion flames.

In addition we must include the appropriate boundary conditions.

Without losing much generality we can state as boundary conditions for the temperature and mass fractions that they be constants at some surfaces or zones of the flow field.

For example, on some surface or region at the fuel side of the flame — the fuel exit —

$$K_i = K_{if} \quad , \quad T = T_f$$

and

$$K_i = K_{io} \quad , \quad T = T_0 \tag{12}$$

on some surface or region far from the flame on the oxidizer side of the flame.

II.6. *Dimensionless Form of the Equations.*

Let us introduce the following non-dimensional variables

$$\vec{x}=L\vec{x}^* \quad,, \quad \vec{v}=U\vec{v}^* \quad,, \quad \rho=\rho_0\rho^* \quad,, \quad p=\rho_0 U^2 p^*$$
$$T=T_0+\frac{q}{c_p}T^* \quad,, \quad \mu=\mu_0\mu^* \quad,, \quad Re=\frac{\rho_0 U L}{\mu_0} \quad,, \quad Sc=\frac{\mu}{\rho D}$$
[13]

Re is the non-dimensional Reynolds number, and Sc is the Schmidt number that will be assumed to be constant and equal to the Prandtl number.

Subscripts $_0$ and $_F$ will indicate boundary conditions far from the flame, on the oxidizer and fuel side of the flame respectively.

The characteristic length L and velocity U are some overall characteristic magnitudes.

In terms of these non-dimensional variables the governing equations take the form.

$$\left|\frac{p_0}{\rho_0 U^2}\right|p^*=\rho^*\left(1+\left|\frac{q}{c_p T_0}\right|T^*\right)$$

$$\nabla^*\cdot(\rho^*\vec{v}^*)=0$$

$$\vec{v}^*\cdot\nabla^*v^*=-\frac{1}{\rho^*}\nabla^*p^*+\left|\frac{1}{Re}\right|\frac{1}{\rho^*}\nabla^*\cdot\sigma^*$$

$$\vec{v}^*\cdot\nabla^*K_i=\left|\frac{1}{Re\,Pr}\right|\frac{1}{\rho^*}\nabla^*\cdot(\mu^*\nabla^*K_i)+\left|\frac{L}{U t_c}\right|\left(\frac{w_i}{\rho}\right)^*$$

$$\vec{v}^*\cdot\nabla^*T^*=\left|\frac{1}{Re\,Pr}\right|\frac{1}{\rho^*}\nabla^*\cdot(\mu^*\nabla^*T^*)-\left|\frac{L}{U t_c}\right|\left(\frac{w_i}{\rho}\right)^*+\left|\frac{U^2}{q}\right|\vec{v}^*\cdot\nabla^*p^*+\left|\frac{U^2}{q Re}\right|\frac{1}{\rho^*}\sigma^*:\nabla^*\vec{v}^*$$
[14]

Here

$$\sigma^*=\sigma\left|\frac{L}{U\mu_0}\right| \quad \text{and} \quad \left(\frac{w_i}{\rho}\right)^*=t_c\left(\frac{w_i}{\rho}\right)$$

where

$$t_c^{-1}=b\cdot\left(\frac{p_0}{RT_f}\right)\exp\left(-\frac{E}{RT_f}\right)$$
[15]

T_f will be the adiabatic temperature of the flame

$$T_f=\frac{q}{c_p}\cdot\frac{K_{2a}(T_F^*+K_{1F})}{K_{2a}+\nu K_{1F}}$$

as we shall see later. Then t_c is a characteristic chemical time, such that $(w_i/\rho)^*$ will be of order unity if the mass fractions are not small and the temperature is close to the adiabatic flame temperature.

III. DISCUSSION OF THE EQUATIONS AND LIMITING CASES

III.1. *General Discussion.*

By choosing appropriately the characteristic magnitudes, the non-dimensional factors and terms in equation [14] should be of order unity except, at most, at regions such as boundary layers, shock waves, free mixing layers. In these regions the functions $\vec{v}$, K_i, T or their derivatives may change very rapidly. If such layers do not exist, or in any other region, the relative importance of the different terms in equations [14] is measured by the values of the non-dimensional parameters

$$\frac{1}{Re} \quad , \quad \frac{L}{U\,t_c} \quad , \quad \frac{U^2}{q} \quad , \quad \frac{U^2}{q}\frac{1}{Re} \quad , \quad Pr \sim 1.$$

This is not exactly true for the term $(L/U\,t_c)\,(w_i/\varphi^*)$ because of the large variations of $(w_i/\varphi)^*$ with temperature and mass fractions.

From equations [6b] and [9] we deduce

$$\vec{v}^*\cdot\nabla^*(K_1 - K_2/\nu) = \left|\frac{1}{Re\,Pr}\right|\frac{1}{\varphi^*}\nabla^*\cdot\{\mu^*\nabla^*(K_1 - K_2/\nu)\}. \tag{16}$$

Also if $U^2/q \ll 1$ and $(1/Re)(U^2/q) \ll 1$ the energy equation may be written

$$\vec{v}^*\cdot\nabla^*T^* = \left|\frac{1}{Re\,Pr}\right|\frac{1}{\varphi^*}\nabla^*\cdot(\mu^*\nabla^*T^*) - \left|\frac{L}{U\,t_c}\right|\left(\frac{w_i}{\varphi}\right)^*. \tag{17}$$

And if the fuel diffusion equation is added to [17] we obtain

$$\vec{v}^*\cdot\nabla^*(K_1 + T^*) = \left|\frac{1}{Re\,Pr}\right|\frac{1}{\varphi^*}\nabla^*\cdot\{\mu^*\nabla^*(K_1 + T^*)\}. \tag{18}$$

If the form [17] of the energy equation is used, and taking into account the diffusion equations, the function

$$\varphi = T^* + \frac{K_{2o} - K_{2F} - \nu T_F^*}{K_{2o} - K_{2F} + \nu(K_{1F} - K_{1o})}\,K_1 + \frac{K_{1F} - K_{1o} + T_F^*}{K_{2o} - K_{2F} + \nu(K_{1F} - K_{1o})}\,K_2$$

satisfies the differential equation

$$\vec{v}^*\cdot\nabla^*\varphi = \left|\frac{1}{Re\,Pr}\right|\frac{1}{\varphi^*}\nabla^*\cdot(\mu^*\nabla^*\varphi) \tag{19}$$

that when solved with the boundary conditions [12] gives

$$\varphi = \frac{K_{2o}K_{1F} - K_{1o}K_{2F} + (K_{2o} - \nu K_{1o})T_F^*}{K_2 - K_{2F} + \nu(K_{1F} - K_{1o})} \tag{20}$$

Solution [20] is independent of the chemical kinetics. There are cases, however, in which the boundary conditions as given in [12] are not known «a priori» because they depend on the chemical kinetics. For example, in the case of a fuel droplet burning in an oxidizing medium, the oxidizer mass fraction at the droplet surface (which is zero for infinite or very large reaction rates) may build up to some unknown value when the reaction rate becomes low.

III.2. *Burke-Schumann Solution.*

For the study of diffusion flames, Burke and Schumann introduced the assumption that the region where w_i/ρ is different from zero is infinitely thin, and $K_1 = 0$ on one side of the flame, and $K_2 = 0$ on the other.

This should be true when $L/U t_c$ is very large. If both K_1 and K_2 were different from zero in a region where the temperature is not low compared with T_f, then $(w_i/\rho)^*$ would be of order unity and the term $[L/U t_c](w_i/\rho)^*$ would be very large compared with

$$\vec{r}^* \cdot \nabla^* K_i \quad \text{and} \quad \left[\frac{1}{Re\,Pr}\right] \frac{1}{\rho^*}\nabla^* \cdot (\rho^* \nabla^* K_i),$$

that are of order unity.

Also if in system [14] we take the limit $L/U t_c \to \infty$, then we obtain the result $(w_i/\rho)^* = 0$. So either $K_1 = 0$ or $K_2 = 0$, and system [14] takes the following form, where $i = 1,3$, $j = 2$ on the fuel side of the flame and $i = 2,3$, $j = 1$ on the oxidizer side of the flame,

$$\left.\begin{array}{c} \left|\dfrac{p_0}{\rho_0 U^2}\right| p^* = \rho^*\left(1 + \left|\dfrac{q}{c_p T_0}\right| T^*\right) \\[2mm] \nabla^* \cdot (\rho^* \vec{r}^*) = 0 \\[2mm] \vec{r}^* \cdot \nabla^* \vec{r}^* = -\dfrac{1}{\rho^*}\nabla^* p^* + \left|\dfrac{1}{Re}\right|\dfrac{1}{\rho^*}\nabla^* \cdot \sigma^* \\[2mm] \vec{r}^* \cdot \nabla^* K_i = \left|\dfrac{1}{Re\,Pr}\right|\dfrac{1}{\rho^*}\nabla^* \cdot (\rho^* \nabla^* K_i) \\[2mm] \vec{r}^* \cdot \nabla^* T^* = \left|\dfrac{1}{Re\,Pr}\right|\dfrac{1}{\rho^*}\nabla^* \cdot (\rho^* \nabla^* T^*) + \left|\dfrac{1}{Re}\dfrac{U^2}{q}\right|\dfrac{1}{\rho^*}\sigma^* : \nabla^* \vec{r}^* + \dfrac{U^2}{q}\dfrac{1}{\rho^*}\vec{v}^* \cdot \nabla^* p^* \\[2mm] K_j = 0 \end{array}\right\} \quad [21]$$

We can use with system [21] the same boundary conditions [12] (*) of system [14], if we allow for discontinuities in the mass and temperature distributions at the zero thickness flame.

In the flame the equations of conservation of mass and energy indicate that, 1) fuel and oxidizer diffuse towards the flame in stoichiometric proportions; 2) that the heat leaving the

(*) K_{10} and K_{20} must be zero if $L/U t_c \to \infty$.

flame due to conduction equals the heat released by the reacting species when reaching the flame. That is

$$\nu \frac{\partial K_1}{\partial n_1} = \frac{\partial K_2}{\partial n_2}$$

$$-\frac{q}{c_p} \frac{\partial K_1}{\partial n_1} = \frac{\partial T}{\partial n_1} + \frac{\partial T}{\partial n_2}$$

[22]

where $\partial/\partial n_1$ and $\partial/\partial n_2$ indicate derivatives normal to the flame surface toward the fuel and oxidizer sides respectively. They must be evaluated at the flame.

The temperature, mass fractions, and therefore the density and velocity, are continuous functions at the flame. For this reason, mass and heat transport by convection is not taken into account when writing the conservation equations through the flame.

By solving the system of equations [21], with boundary conditions [12] and [22], we obtain the Burke-Schumann velocity, mass fractions, and temperature distributions.

In particular, let

$$K_1 - K_2/\nu = f_1(\vec{x})$$

$$K_1 + T^* = f_2(\vec{x})$$

[23]

be the solutions of equations [16] and [18] (valid only for $U^2/q \ll 1$ and $(1/Re)\ U^2/q \ll 1$).

The equation of the flame surface is obtained by writing

$$K_1 = K_2 \quad 0 \quad f_1(\vec{x}) = 0.$$

Also according to [20] at the flame

$$T^* = T_f^* = \frac{(K_{1F} + T_F^*) K_{20}}{\nu K_{1F} + K_{20}}$$

and

$$T_f = T_0 + \frac{q}{c_p} \frac{(K_{1F} + T_F^*) K_{20}}{\nu K_{1F} + K_{20}}.$$

[24]

By writing $K_2 = 0$ on the fuel side of the flame surface and $K_1 = 0$ on the oxidizer side, we obtain the temperature and mass fraction distributions.

$$\begin{array}{ll} K_1 = f_1(\vec{x}) & \\ K_2 = 0 & \text{for } f_1 > 0 \\ T^* = f_2(\vec{x}) - f_1(\vec{x}) & \end{array} \qquad \begin{array}{ll} K_1 = 0 & \\ K_2 = -\nu f_1(\vec{x}) & \text{for } f_1 < 0. \\ T^* = f_2(\vec{x}) & \end{array}$$

[25]

It is interesting to point out that the Burke-Schumann solution satisfies the complete system of equations [14] and also its boundary conditions. This solution is not the correct one, only because the first derivatives of the temperature and mass fraction distributions have discontinuous first derivatives within the flow field.

Solutions [23] of equations [16] and [18] are modified when finite values of $L_i/U\ t_c$ are con-

sidered. The reason for these modifications is that, although reaction rates do not appear explicitly in equations [16] and [18], the variables ρ, $\vec{v}$ and μ that appear in those equations will depend on the reactions rates.

However, we may expect that, for sufficiently large values of $L/U\,t_c$, the reaction zone (or region where $w_i \neq 0$) will be very thin. Hence the Burke-Schumann solution [25], for which the reaction zone has zero thickness, will be a very good approximation in the case of large but finite $L/U\,t_c$. This will be especially true outside of the reaction zone.

Equations [16] and [18], in particular, should remain practically unchanged. This is exactly right when mixing and reaction takes place in constant pressure regions and boundary layers if $\rho\mu$ is assumed to be constant. In such cases equations [16] and [18] as well as the boundary conditions (for large $L/U\,t_c$), will be independent of the reaction rates. The same will happen then to their solution.

Summing up: If the reaction rate is sufficiently large the reaction zone will be very thin compared with any other important length (as for example, the width of the mixing region). Then, in order to obtain the velocity, temperature and mass fraction distributions outside of the reaction zone, i. e., for the study of the external structure of the diffusion flame, we may use the assumption of infinite reaction rates.

IV. STRUCTURE OF THE REACTION ZONE

IV.1. The «Chemical Boundary Layer».

The fact that in the limiting case of infinite reaction rates the thickness of the reaction zone is zero, and that the first derivatives of K_i and T normal to the flame are discontinuous there, suggests that for large, although finite, $L/U\,t_c$:

a) The thickness of the reaction zone will be small.

b) The diffusion terms

$$\frac{1}{\rho}\,\frac{\partial}{\partial n}\left(\frac{\mu}{\mathrm{Pr}}\,\frac{\partial K_i}{\partial n}\right) \quad \text{and} \quad \frac{1}{\rho}\,\frac{\partial}{\partial n}\left(\frac{\mu}{\mathrm{Pr}}\,\frac{\partial T}{\partial n}\right)$$

will balance the chemical production terms w_i/ρ, these terms being very large compared with all the other terms of the equations. (Here $\partial/\partial n$ indicates differentiation normal to the flame).

In other words, for large values of the chemical reaction rates the reaction zone will be a very thin region or «chemical boundary layer». There, due to the rapidly varying gradients of temperature and mass fractions normal to the flame, mass diffusion and heat conduction normal to the flame constitute the only transport mechanism required to balance the chemical production terms. Transport by diffusion or conduction in other directions or convection may be neglected within the reaction zone.

In order to show this, let us assume that we know the Burke-Schumann solution [25]. Hence, we know the flame surface location for infinite $L/U\,t_c$, and therefore the approximate location of the flame region for large $L/U\,t_c$.

For simplicity we will limit ourselves to the two-dimensional case. The results, however, are completely general. We shall write the equations of motion, and mass and energy conservation equations in a curvilinear system of coordinates. In this system, see Fig. 1,

x will be the distance measured along the flame surface, as determined by the Burke-Schumann solution. The distance normal to this surface will be indicated by y; u and r will be the velocity components in the x and y directions; $1/K$ is the radius of curvature of the flame at point x. Limiting ourselves to a region where Ky is small compared with 1 the line element has components $(1 + Ky)dx$ and dy, and the equations are as follows:

Continuity for the mixture

$$\frac{1}{1+Ky}\frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial y}(\rho r) + \frac{K\rho r}{1+Ky} = 0.$$

Equations of motion

$$\rho\left|\frac{u}{1+Ky}\frac{\partial u}{\partial x} + r\frac{\partial u}{\partial y} + \frac{Kur}{1+Ky}\right| = -\frac{1}{1+Ky}\frac{\partial p}{\partial x} + F_u$$

$$\rho\left|\frac{u}{1+Ky}\frac{\partial v}{\partial x} + r\frac{\partial r}{\partial y} - \frac{Ku^2}{1+Ky}\right| = -\frac{\partial p}{\partial y} + F_r$$

where

$$F_u = \frac{1}{1+Ky}\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} + \frac{2K\sigma_{xy}}{1+Ky}$$

$$F_r = \frac{1}{1+Ky}\frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + \frac{K(\sigma_{yy} - \sigma_{xx})}{1+Ky}$$

$$\sigma_{xx} = 2\mu\left(\frac{1}{1+Ky}\frac{\partial u}{\partial x} + \frac{Kr}{1+Ky}\right) - \frac{2}{3}\mu\nabla\cdot\vec{r}$$

$$\sigma_{yy} = 2\mu\frac{\partial r}{\partial y} - \frac{2}{3}\mu\nabla\cdot\vec{r}$$

$$\sigma_{xy} = \mu\left(\frac{1}{1+Ky}\frac{\partial r}{\partial x} + \frac{\partial u}{\partial y} - \frac{Ku}{1+Ky}\right)$$

$$\nabla\cdot\vec{r} = \frac{1}{1+Ky}\frac{\partial u}{\partial x} + \frac{\partial r}{\partial y} + \frac{Kr}{1+Ky}.$$

Continuity equation for each of the species

$$\frac{u}{1+Ky}\frac{\partial K_i}{\partial x} + r\frac{\partial K_i}{\partial y} = \frac{1}{\rho(1+Ky)}\left\{\frac{\partial}{\partial x}\left|\frac{\mu}{Pr}\frac{1}{1+Ky}\frac{\partial K_i}{\partial x}\right| + \frac{\partial}{\partial y}\left|\frac{\mu}{Pr}(1+Ky)\frac{\partial K_i}{\partial y}\right|\right\} + \frac{w_i}{\rho}.$$

Energy equation

$$\frac{u}{1+Ky}\frac{\partial T}{\partial x} + r\frac{\partial T}{\partial y} = \frac{1}{\rho(1+Ky)}\left\{\frac{\partial}{\partial x}\left|\frac{\mu}{Pr}\frac{1}{1+Ky}\frac{\partial T}{\partial x}\right| + \frac{\partial}{\partial y}\left|\frac{\mu}{Pr}(1+Ky)\frac{\partial T}{\partial y}\right|\right\}\left\{-\frac{q}{c_p}\frac{w_i}{\rho}\right\} +$$

$$+ \frac{1}{\rho c_p}\Phi_r + \frac{1}{\rho c_p}\frac{u}{1+Ky}\frac{\partial p}{\partial x} + \frac{1}{\rho c_p}r\frac{\partial p}{\partial y}$$

where

$$\Phi_r = \mu[2(\varepsilon_{xx}^2 + \varepsilon_{yy}^2) + \varepsilon_{xy}^2 - 2/3(\varepsilon_{xx} + \varepsilon_{yy})^2]$$

and

$$\varepsilon_{xx} = \frac{1}{1+Ky}\frac{\partial u}{\partial x} + \frac{Kv}{1+Ky}$$

$$\varepsilon_{yy} = \frac{\partial v}{\partial y}$$

$$\varepsilon_{xy} = \frac{1}{1+Ky}\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} - \frac{Ku}{1+Ky}$$

Now let L and U be overall characteristic length and velocity. Let δ_c and δ_m be the thicknesses of the reaction zone and of the mixing region respectively. We could show that for low Reynolds number, $\delta_m \sim L$, while $\delta_m \sim \sqrt{D_0 L/U}$ for large Reynolds numbers.

The mass fractions just at the outer edge of the reaction zone will be of order δ_c/δ_m. The same order of magnitude will be valid inside of the reaction zone.

Let us now introduce the non-dimensional variables x/L, y/δ_c, $K_i \delta_m/\delta_c$, $(w_i/\rho) t_c (\delta_m/\delta_c)^2$, by stretching the coordinates, mass fractions and reaction rates, so as to make the non-dimensional factors and terms of order unity within the reaction zone. For the remaining variables we may use the same non-dimensional variables used in section II.

We will write the governing equations in terms of these non-dimensional variables. Now, if the terms accounting for the conduction and diffusion normal to the flame are going to be of the order of the chemical production term, $\delta_c^2 \sim \delta_m D_0 t_c$.

If we now take, in the energy and diffusion equations, the limit $\delta_c/\delta_m \to 0$, most of the terms in these equations drop out. We are left with the following differential equations:

$$\frac{1}{\rho}\frac{\partial}{\partial y}\left(\frac{\mu}{Pr}\frac{\partial K_i}{\partial y}\right) = \frac{w_i}{\rho} \qquad [26]$$

$$\frac{1}{\rho}\frac{\partial}{\partial y}\left(\frac{\mu}{Pr}\frac{\partial T}{\partial y}\right) = -\frac{q}{c_p}\frac{w_1}{\rho} \qquad [27]$$

that we have written in dimensional form.

From the momentum equation we deduce that the variations of pressure across the reaction zone are of order δ_c/L.

Hence we may assume, when writing the equation of state, that the pressure is constant across the reaction region and equal to the value obtained at the flame with the Burke-Schumann assumption.

Therefore in addition to the above equations for K_1, K_2, and T we have the equation

$$p(x) = \rho T R/M$$

where $p(x)$ is a known function of x.

Also

$$w_2 = w_1 = b \cdot [p(x) R T] \exp[-E/RT] K_1 K_2 \qquad [29]$$

or we may use the general expression [7] for w_i as is done in appendix A.

No derivatives with respect to x appear in system [26] to [29]. Therefore these equations may be solved as ordinary differential equations in which x stands as a parameter.

As boundary conditions we will write that when $y \to \pm \infty$ the temperature and mass fraction distributions coincide with those obtained by assuming the reaction rate to be infinite.

IV.2. *The Solution of the Chemical Boundary Layer Equations.*

By introducing the new variable $y_1 = \int_0^y (\varrho/\varrho_0)\, dy$, if we assume that $\varrho\mu = \varrho_0\mu_0$, equations [27] and [28] may be written

$$\frac{d^2 K_i}{d y_1^2} = \frac{1}{D_0} \frac{w_i}{\varrho} \tag{30}$$

$$\frac{d^2 T^*}{d y_1^2} = \frac{1}{D_0} \frac{w_1}{\varrho} . \tag{31}$$

From equations [30] if we take into account that $w_2 = \nu w_1$ we get

$$K_1 - K_2 \nu = A_1 y_1 + B_1. \tag{32}$$

Similarly, from [30] and [31] we obtain

$$K_1 - T^* = A_2 y_1 + B_2 \tag{33}$$

$$K_2 \nu + T^* = A_3 y_1 + B_3. \tag{34}$$

Relations [32] to [34] are independent of the chemical reaction rates. However, they are only valid within the reaction zone. The constants A_i, B_i must be chosen so that these relations coincide with the similar relations obtained from the Burke-Schumann solution, at least for low values of y_1. Then, relations [33] and [34] may be written,

$$K_1 = T_f^* \left[1 + \theta + \frac{\nu}{K_{20}} \frac{\dot{m}}{\varrho_0 D_0} y_1 \right]$$
$$K_2 = \nu T_f^* \left[1 + \theta - \left(\frac{1}{T_f^*} + \frac{\nu}{K_{20}} \right) \frac{\dot{m}}{\varrho_0 D_0} y_1 \right] \tag{35}$$

Where

$$\theta = T^* + T_f^* \quad , \quad T_f^* = \frac{K_{20}(T_f^* + K_{10})}{K_{20} + \nu K_{10}} \quad \text{and} \quad \dot{m}(x) = \left[\varrho D \frac{\partial K_1}{\partial y} \right]_{y=0} ,$$

sometimes called flame strength, is the mass rate of fuel comsumption per unit flame surface. Also we may write $\varrho_0 D \cdot \dot{m}(x) = \delta_m(x)$ where $\delta_m(x)$ is a mixing layer thickness.

Now, by using expression [6a] for the fuel production rate, equation [31] takes the following form:

$$\frac{d^2\theta}{dy_1^2} = -\frac{\nu T_f^*}{D_0 t_c}\frac{p}{p_0}\frac{1+\theta_0}{\theta_0+\theta}\exp\left\{-\frac{\theta_a}{1+\theta_0}\frac{1-\theta}{\theta_0+\theta}\right\}\left[1-\theta+\frac{\nu}{K_{20}}\frac{y_1}{\delta_m}\right]\left[1-\theta-\left(\frac{1}{T_f^*}-\frac{\nu}{K_{20}}\right)\frac{y_1}{\delta_m}\right] \quad [36]$$

where $\theta_0 = c_p T_0/q$ and $\theta_a = E c_p/R q$ is the non-dimensional activation energy of the reaction.

By solving equation [36] with the boundary conditions $K_2 = 0$ for $y_1 \to \infty$ and $K_1 = 0$ for $y_1 \to -\infty$, we obtain the temperature distribution within the reaction zone.

If the reaction rate is sufficiently large, the temperature will not deviate appreciably, within the reaction zone, from its limiting value (when $t_c \to 0$) $\theta = 1$ at $y_1 = 0$.

Then a good approximate solution of [36] may be obtained by substituting the factor

$$\frac{1}{\theta_0 + \theta}\exp\left\{-\frac{\theta_a}{1+\theta_0}\frac{1-\theta}{\theta_0+\theta}\right\}$$

by its value at $y_1 = 0$. Let $\theta = \theta_c(x)$ for $y = 0$. Then we approximate equation [36] by

$$\frac{d^2\theta}{dy_1^2} = -\frac{\nu T_f^*}{D_0 t_c}\frac{p}{p_0}\frac{1+\theta_0}{\theta+\theta_c}\exp\left\{-\frac{\theta_a}{1+\theta_0}\frac{1-\theta_c}{\theta_0+\theta_c}\right\}\left[1-\theta+\frac{\nu}{K_{20}}\frac{y_1}{\delta_m}\right]\left[1-\theta-\left(\frac{1}{T_f^*}-\frac{\nu}{K_{20}}\right)\frac{y_1}{\delta_m}\right]. \quad [37]$$

This we may write in the form

$$\frac{d^2\beta}{dz^2} = \beta^2 - z^2 \quad [38]$$

and the boundary conditions are:

$$\beta + z = 0 \quad \text{for} \quad z \to +\infty.$$

Here

$$\beta = \sqrt{A}\left[1 - \theta + \left(\frac{\nu}{K_{20}} - \frac{1}{2T_f^*}\right)\frac{y_1}{\delta_m}\right] \quad , \quad z = \frac{y_1}{\delta_c}, \quad [39]$$

where

$$A = 4\nu T_f^{*3}\frac{\delta_m^2}{D_0 t_c}\frac{p}{p_0}\frac{1+\theta_0}{\theta_0+\theta_c}\exp\left\{-\frac{\theta_a}{1+\theta_0}\frac{1-\theta_c}{\theta_0+\theta_c}\right\} \quad [40]$$

$$\delta_m = \frac{\theta_0 D_0}{m} \quad , \quad \delta_c^3 = \delta_m D_0 t_c \frac{2}{\nu}\frac{p_0}{p}\frac{\theta_0+\theta_c}{1+\theta_0}\exp\left\{\frac{\theta_a}{1+\theta_0}\frac{1-\theta_c}{\theta_0+\theta_c}\right\}. \quad [41]$$

Equation [39] was solved numerically (15). Its solution

$$\beta = \beta(z), \quad [38a]$$

is represented in Fig. 2 with a solid line. In particular $\beta(o) = 0.866$. An approximate solution is presented in Appendix A.
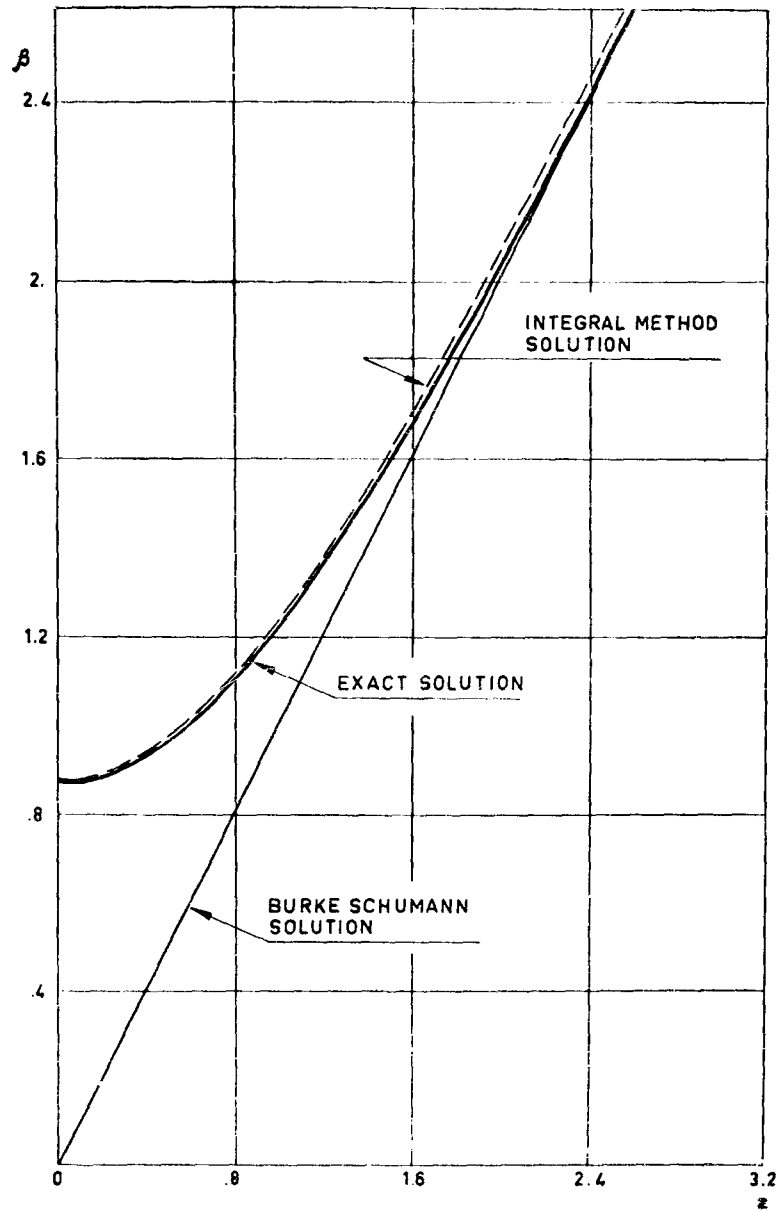
Fig. 2. Universal temperature distribution function.

Fig. 3 shows the variation with z of $\beta^2 - z^2$, which is proportional to the fuel mass consumption rate per unit volume. For $z = 3.2$ its value is roughly one per cent of its maximum value at $z = 0$. Hence we may conclude that the thickness of the reaction zone or chemical boundary layer is of the order of $6\,\delta_c$.

According to [38a] the temperature at the ideal (Burke-Schumann) flame surface position, $y_i = 0$, is given by the following relation

$$\theta_c = 1 - \frac{0.87}{\sqrt[3]{A}} .\qquad [42]$$

A first approximation for θ_c is obtained by writing $\theta_c = 1$ when evaluating A. Then θ_c is given by

$$\theta_c = 1 - \frac{0.87}{\sqrt[3]{A_0}} .\qquad [43]$$

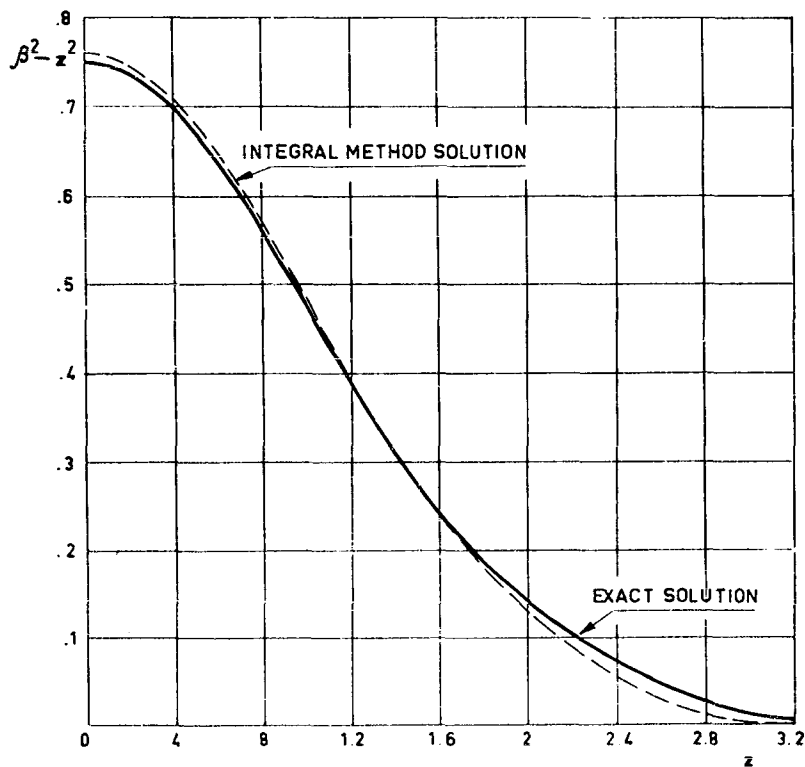

Fig. 3. — Chemical mass production rate distribution.

where

$$A_0 = 4 \nu T_f^{*3} \frac{p}{p_0} \frac{\delta_m^2}{D_0 t_c} = 4 \nu T_f^{*3} \frac{p}{p_0} \frac{\rho_0^2 D_0}{\dot{m}^2 t_c}. \qquad [44]$$

A second approximation for θ_c valid for values of $\theta_c > 0.8$ is

$$\theta_c = 1 - \frac{0.87}{\sqrt[3]{A_0}} \left[1 - \frac{\theta_a - 1 - \theta_0}{3(1 - \theta_0)^2} \frac{0.87}{\sqrt[3]{A_0}} \right]. \qquad [45]$$

Similarly

$$\delta_c \delta_m = \frac{2 T_f^*}{0.87} (1 - \theta_c). \qquad [46]$$

IV.3. *Discussion of the solution.*

Relation [45] shows that deviations of the temperature from its asymptotic Burke-Schumann value $\theta_c = 1$ depend on the parameter A_0. This parameter incorporates both the chemical kinetic parameters (through the value of the characteristic chemical time t_c) and the fluid mechanical parameters (through the mixing time $t_m(x) = \delta_m^2(x) D_0$). $A_0 \sim t_m/t_c$.

The obvious result is that the deviations of the temperature and mass fractions from their limiting asymptotic values increase with decreasing values of the ratio t_m/t_c. Now t_m is inversely proportional to the fuel rate of supply to the flame $\dot{m}$. Hence we deduce that by increasing the fuel rate of supply, the flame temperature will decrease.

The initial fuel and oxidizer mass fractions influence the results through the factor T_f^{*3} that appears in [44]. By diluting the fuel or the oxidizer we get larger deviations from the Burke-Schumann result.

Relation [46] indicates that the thickness of the reaction region decreases with increasing values of the mass rate of fuel supply.

For this chemical boundary layer scheme to be valid $\delta_c \delta_m$ must be small compared to unity, hence the same criterion may be used for the validity of the Burke-Schumann assumption and solution, and for the validity of the chemical boundary layer solution.

Obviously, the most important characteristics of the chemical boundary layer solution and those of the Burke-Schumann solution coincide. For example, flame location and the quantity of fuel burning per unit flame area are the same in both solutions. The chemical boundary layer solution, however, gives a finite thickness for the reaction zone, and a small correction to the temperature and mass fraction distributions. This correction can be evaluated very easily and accurately in terms of the chemical kinetic parameters of the reaction. So, the chemical boundary layer solution can be of help for the study of chemical kinetics by means of experimentation in diffusion flames (12), (23).

The parameter A_0 that measures the deviations from the infinite reaction rate solution, may be used for the determination of an extinction criterion. This is supported by the following reasons:

a) Due to the high values of the activation energy of many of the chemical reactions, the chemical production term is very sensitive to temperature variations. This accounts for the fact that flame extinction occurs in a rather sharply defined way. This may also be due to the existence of some ignition temperature for the reaction.

b) The concept of an overall reaction rate is not in general valid through a large temperature range. Then, the idea of solving the complete exact equations, for obtaining an «exact» extinction criterion, loses part of its interest if use has to be made of some assumed overall reaction rate expression throughout the whole temperature range.

c) The chemical boundary layer solution, although it cannot explain extinction except in a qualitative way, can provide a criterion for extinction not to occur if the overall reaction rate is known to be valid in a given temperature range.

Whenever the parameter A_0 is sufficiently low as to make $T_c \sim 0.8 T_f$ (and this occurs for, roughly, $A_0 \sim 80$), the thickness of the reaction region begins to be comparable with the thickness of the mixing region. Then the rate of fuel consumption begins to diminish and hence T_c will begin to decrease even faster with decreasing A_0.

Therefore, $A_0 \sim 80$ may be used as an approximate extinction criterion as well as a criterion for the validity of the Burke-Schumann solution.

We have seen that $A_0 \sim \rho_0^2 D_0 / \dot{m}^2 t_c$. Now, this same parameter appears in the theory of premixed laminar flames. There it takes a value of the order of 100, that depends on the initial mass fractions and energy of activation of the reaction (24), when $\dot{m}$ is substituted by the fuel consumption rate G per unit area. Therefore an «approximate» relation may be established (9), (10) between the value of $\dot{m}$ at extinction (maximum flame strength) and G:

$$\dot{m}_{ext} \sim G.$$

V. THE EXTERNAL STRUCTURE OF LAMINAR DIFFUSION FLAMES

V.1. *Large Reynolds Number Case. Inviscid Equations.*

The chemical boundary layer equations, governing the temperature and mass fraction distributions within the reaction zone, have been solved in the most general case. However, for the detailed evaluation of the solution we must know some parameters appearing there. They include the mass rate $\dot{m}$ of fuel consumption per unit flame surface, and the ideal flame location.

In order to evaluate these parameters as well as the mass fraction and temperature distributions outside of the reaction zone, the Burke-Schumann solution must be obtained first.

As mentioned in the introduction this solution has been obtained in some particular cases. Unfortunately, even when using the Burke-Schumann assumption of infinite reaction rates, the resulting system of equations [21] and boundary conditions [12] and [22] is so complicated that only a few approximate solutions exist.

Marble and Adamson (17) have pointed out that a number of important combustion problems may be investigated analytically with the help of boundary layer approximations. Most of the solutions so far obtained make use of these approximations. These may be used whenever the Reynolds number, based on some overall dimension of the flow field, is sufficiently large.

We will show here that, by using some additional assumptions, a fairly simple solution of the Burke-Schumann mixing problem is obtained.

If in system [21] we take the limit Re $\to \infty$, we obtain the following system of differential equations, that we shall write in dimensional form:

$$p = \rho T R/M$$

$$\left. \begin{aligned}
\nabla \cdot (\rho \vec{r}) &= 0 \\
\vec{r} \cdot \nabla \vec{r} &= -\frac{1}{\rho} \nabla p \\
\vec{r} \cdot \nabla K_i &= 0 \\
\vec{r} \cdot \nabla T &= \frac{1}{\rho c_p} \vec{r} \cdot \nabla p
\end{aligned} \right\} \qquad [47]$$

The boundary conditions [22] cannot be retained because, in the process of taking the limit Re $\to \infty$, we dropped the higher derivatives in the equations.

However the boundary conditions [12] can be satisfied if we allow for the existence of discontinuities in temperature, mass fractions, density, and velocity at some stream surface. The position of this surface is determined by requiring that all the boundary conditions [12] be satisfied.

If we consider only low Mach number flows, then:

1) The density, temperature and mass fractions will be constant, although possibly with different values, on each side of the discontinuity surface. See Fig. 1.

2) Equations [47] reduce to the system

$$\left. \begin{aligned}
\nabla \cdot \vec{r} &= 0 \\
\vec{r} \cdot \nabla \vec{r} &= -\frac{1}{\rho} \nabla p
\end{aligned} \right\} \qquad [48]$$

and tangential discontinuities of $\vec{r}$ are allowed for at some surface, so as to satisfy the required boundary conditions on $\vec{r}$. The pressure must, of course, be continuous at the surface.

As an example, the solution of this problem for the low speed source flow is presented in Appendix C.

V.2. Mixing Layer Equations.

For large but finite Re, the ideal discontinuity surface is substituted by a thin mixing layer with the same approximate location. Although the discontinuities in the temperature, mass fractions, etc., no longer exist, the derivatives of these variables normal to the mixing layer will be very large compared to the derivatives in the surface direction:

In order to study the structure of the mixing region, we will write the system [21] in boundary layer coordinates. Then we can obtain the mixing layer equations by using the well known boundary layer limiting process.

Limiting ourselves to the two-dimensional or axially-symmetric low Mach number flow cases, we will write these equations in the form given by Lees (25).

$$\eta = \frac{\rho_0 u_0}{\sqrt{2\xi}} \int_0^Y r^k (\rho/\rho_0)\, dY \quad \Bigg\}$$

$$\xi = \int_0^X \rho_0 \mu_0 u_0 r^{2k}\, dX \qquad \Bigg\} \qquad [49]$$

where $k=0$ for two-dimensional flows and $k=1$ for axially-symmetric flows; $u_0(x)$ is the velocity at the oxidizer side, just outside of the mixing layer.

By introducing the stream function Ψ such that

$$\rho u r^k = \frac{\partial \Psi}{\partial Y} \quad , \quad \rho v r^k = -\frac{\partial \Psi}{\partial X}. \qquad [50]$$

The continuity equation is automatically satisfied. Let

$$\Psi(\xi, \eta) = \sqrt{2\xi}\, f(\eta, \xi). \quad \text{Then} \quad u/u_0 = f'(\eta, \xi) \qquad [51]$$

where the primes denote differentiation with respect to η. We will assume $\rho \mu = \rho_0 \mu_0$. Then the mixing layer equations take the form

$$f''' + ff'' + \frac{2\xi}{u_0}\frac{d u_0}{d\xi}\, [T/T_0 - (f')^2] = \text{t.i.d.}\,\xi \quad \Bigg\}$$

$$K_i'' + \Pr f K_i' = \text{t.i.d.}\,\xi \quad , \quad K_j = 0 \qquad \Bigg\} \qquad [52]$$

$$T'' + \Pr f T' = \text{t.i.d.}\,\xi \qquad \Bigg\}$$

Where $i=1,3;\ j=2$ on the fuel side of the flame, and $i=2,3;\ j=1$ on the other side. The t.i.d. ξ's in the right hand side of the equations indicate terms involving derivatives with respect to ξ.

As boundary conditions we may write

$$\nu \left(\frac{\partial K_1}{\partial \eta}\right)_{\eta_f} = -\left(\frac{\partial K_2}{\partial \eta}\right)_{+\eta_f} = 0 \quad \Bigg\}$$

$$\frac{q}{c_p}\left(\frac{\partial K_1}{\partial \eta}\right)_{\eta_f} = \left(\frac{\partial T}{\partial \eta}\right)_{-\eta_f} - \left(\frac{\partial T}{\partial \eta}\right)_{+\eta_f} \quad \Bigg\} \qquad [53a]$$

Where $\eta_f(\xi)$ gives the ideal flame position.

In addition

$$f' = 1 \quad , \quad K_2 = K_{20} \quad , \quad T = T_0 \quad \text{for} \quad \eta \to \infty \quad \Big\}$$

$$f' = u_r/u_0 \quad , \quad K_1 = K_{11} \quad , \quad T = T_r \quad \text{for} \quad \eta \to -\infty \quad \Big\} \qquad [53b]$$

For the solution of the above mixing problem a third boundary condition for f is required. This should be derived from the compatibility condition of the higher order

approximation (26). However, for our purposes we may write as third boundary condition $f(0, \xi) = 0$, because the only effect of changing the value of $f(0, \xi)$ is a displacement of the mixing layer in the Y direction.

V.3. Local Similarity Approximation.

As the boundary conditions are independent of ξ, the functions f, K_i and T would be functions only of η, and similarity would exist, if the pressure gradient parameter $(2\xi/u_0) d u_0/d\xi$ were constant.

This occurs at the stagnation point where the parameter has the values 1/2, for the axially-symmetric case, and 1 for the two-dimensional one.

Similarity also exists in the constant pressure case corresponding to the mixing of two parallel streams. In this case the pressure gradient term is obviously zero. The local similarity approximation may be used when $(2\xi/u_0) d u_0/d\xi$ is a slowly varying function of ξ. Then we may neglect the t.i.d.ξ's in the right hand side of equation [52]. The resulting system of differential equations may then be integrated as a system of ordinary differential equations.

It is interesting to point out that the factor $[T/T_0 - (f')^2]$ in the pressure gradient term approaches zero at both edges of the mixing layer. The neglect of the pressure gradient term is similar to the neglect of free convection in diffusion flames.

The pressure gradient term is neglected, without much justification, by Spalding when studying the opposed jet diffusion flame (12).

If our main purpose is assessing the effects of chemical kinetics in diffusion flames, only an approximate analytical solution of the equations is required.

This may be obtained easily if we neglect the pressure gradient term in the momentum equation [52]. Then it reduces to the Blassius equation

$$f''' + f f'' = 0 \qquad [54]$$

with the boundary conditions

$$f(o) = 0, \qquad f'(\infty) = 1, \qquad f'(-\infty) = \lambda = u_{-}/u_0.$$

An approximate analytical solution of this equation is given in Appendix B. The first approximation is

$$f' = u/u_0 = \frac{1 + \lambda}{2} + \frac{1 - \lambda}{2} \, \mathrm{erf}\left(\frac{1 + \lambda}{2} \eta\right). \qquad [55]$$

From equations [52] we deduce the following system of equations

$$(K_1 - K_2 \cdot)'' + \mathrm{Pr} f (K_1 - K_2 \cdot)' = 0 \qquad [56]$$

$$(K_1 - T^*)'' + \mathrm{Pr} f (K_1 - T^*)' = 0 \qquad [57]$$

Taking into account the boundary conditions [53 b] we obtain, if $\Pr \ 1$,

$$\frac{(K_2/\nu - K_1) - (K_{20}\,\nu - K_{1F})}{K_{1F} \cdot K_{20}\,\nu} = \text{erf}\left(\left|\frac{1+\lambda}{2}\right|\,\gamma_i\right)$$

$$\frac{T^* + K_1}{T_F^* + K_{1F}} = \frac{1}{2}\left[1 - \text{erf}\left(\left|\frac{1+\lambda}{2}\right|\,\gamma_i\right)\right].$$ [58]

And the boundary conditions at γ_{if} are satisfied identically.

The flame surface is located at the point $\gamma_i = \gamma_{if}$ where

$$\text{erf}\left(\left|\frac{1+\lambda}{2}\right|\,\gamma_{if}\right) = \frac{K_{1F} - K_{20}/\nu}{K_{1F} + K_{20}\,\nu}$$ [59]

and

$$\dot{m} = \left|\rho D \frac{\partial K_1}{\partial y}\right|_{\gamma_{if}} \quad \frac{\rho_0^2 D_0 u_0 r^k}{|2\xi|}\left(\frac{\partial K_1}{\partial \gamma_i}\right)_{\gamma_{if}} = \frac{\rho_0^2 D_0 u_0 r^k}{|2\xi|}(K_{1F} + K_{20}/\nu)\left|\frac{1+\lambda}{2}\right|\frac{1}{\pi}\,e^{-\frac{1+\lambda}{4}\gamma_{if}^2}$$ [60]

So

$$\frac{1}{\delta_m(K)} = \frac{\rho_0 u_0 r^k}{|2\xi|}(K_{1F} + K_{20}\,\nu)\left|\frac{1+\lambda}{2}\right|\frac{1}{\pi}\exp\left\{-\frac{1+\lambda}{4}\gamma_{if}^2\right\}.$$ [61]

The parameter A_0, measuring the deviations from the Burke-Schumann solution, can now be evaluated. Also the temperature and mass fraction distributions outside of the reaction zone may be obtained from [57] and [58] by putting $K_1 = 0$ for $\gamma_i > \gamma_{if}$ and $K_2 = 0$ for $\gamma_i < \gamma_{if}$.

In the particular case $\lambda = 1$, we get $f' = 1$, and the equations may be solved even for $\Pr \neq 1$. We obtain

$$K_1 - K_2\,\nu = K_{1F} - (K_{1F} + K_{20}\,\nu)\frac{1}{2}\left[1 + \text{erf}\left|\frac{\Pr}{2}\,\gamma_i\right|\right]$$

$$T^* + K_1 = (T_F^* + K_{1F})\frac{1}{2}\left[1 - \text{erf}\left|\frac{\Pr}{2}\,\gamma_i\right|\right]$$

$$\dot{m} = \frac{\rho_0^2 D_0 u_0 r^k}{|2\xi|}(K_{1F} + K_{20}\,\nu)\left|\frac{\Pr}{2\pi}\,e^{\frac{\Pr}{2}\gamma_{if}^2}\right.$$

$$\text{erf}\left|\frac{\Pr}{2}\,\gamma_{if}\right| = \frac{K_{1F} - K_{20}\,\nu}{K_{1F} + K_{20}\,\nu}$$ [62]
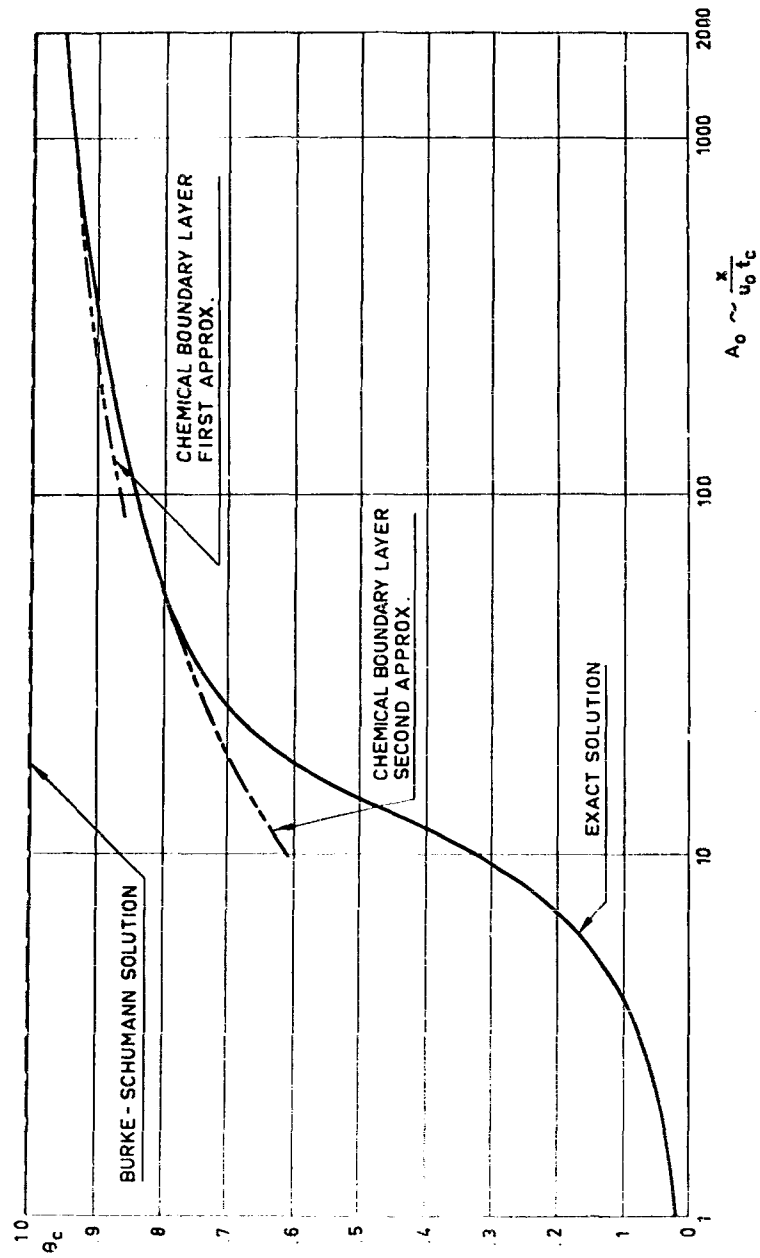
Fig. 4. — Temperature at the Burke-Schumann flame surface as a function of the distance to the initial mixing point.
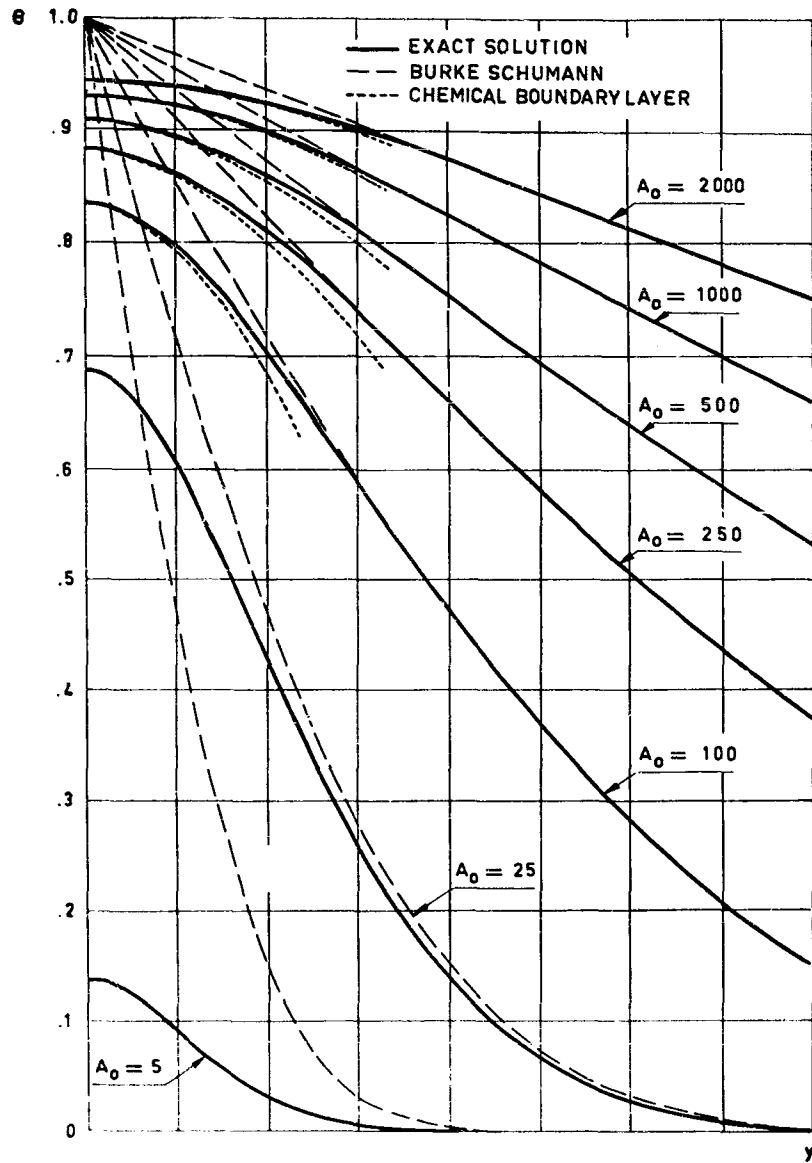
Fig. 5. Temperature distribution profiles at several distances to the initial mixing point.
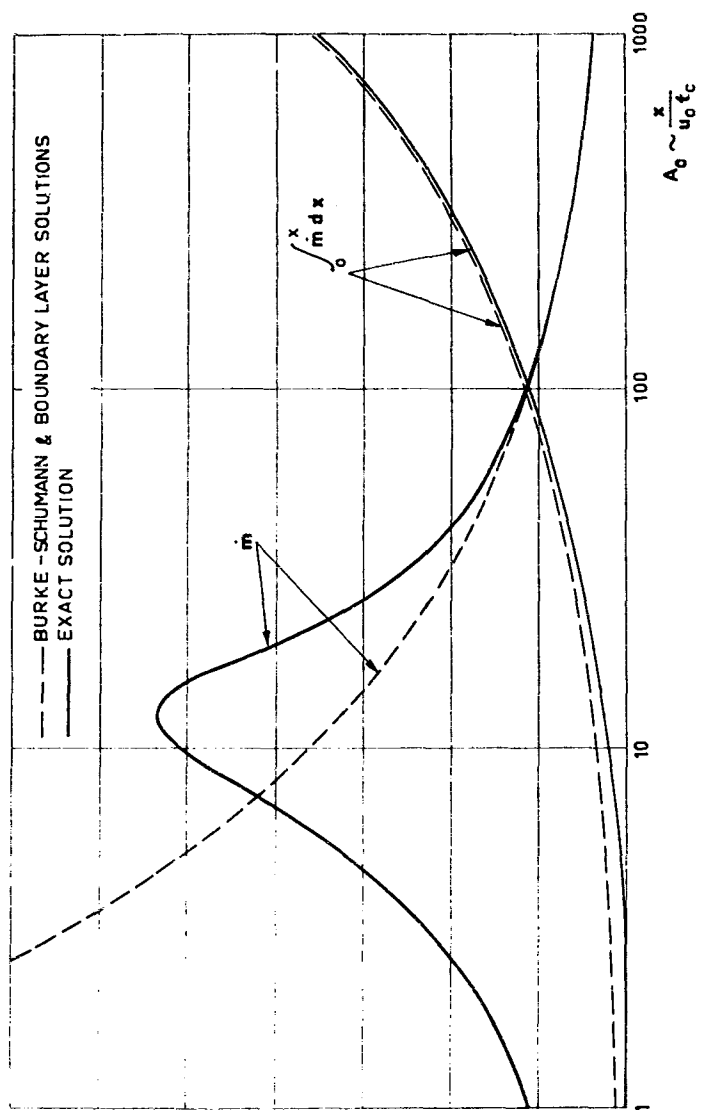
Fig. 6. Total fuel mass consumption, and mass consumption rate per unit flame surface.

V.4. *Particular Cases.*

In particular let us consider:

a) Axially-symmetric stagnation point

$$\frac{\dot{m}}{\rho_0 U_\infty} = \left| \frac{U_\infty R_0}{D_0} \quad (K_{1F} + K_{20}\nu) \right| \frac{3(1+\lambda)}{4\pi} \quad \exp\left\{ -\frac{1+\lambda}{4} \eta_f^2 \right\}. \qquad [63]$$

And according to [44]

$$A_0 = R_0 U_\infty t_c. \qquad [64]$$

b) Mixing of two parallel streams

$$\frac{\dot{m}}{\rho_0 U_0} = \left| \frac{D_0}{U_0 x} \quad (K_{1F} + K_{20}\nu) \right| \frac{1+\lambda}{2|2\pi} \exp\left\{ -\frac{1+\lambda}{4} \eta_f^2 \right\} \qquad [65]$$

$$A_0 = 4\nu T_f^{*3} \frac{x}{U_0 t_c} \frac{8\pi}{1+\lambda} (K_{1F} + K_{20}\nu)^{-2} \exp\left\{ \frac{1+\lambda}{4} \eta_f^2 \right\}. \qquad [66]$$

Therefore

$$A_0 = x U_0 t_c. \qquad [67]$$

In reference (15) a numerical integration of the equations for the mixing and simultaneous chemical reaction of two parallel streams of fuel and oxidizer, moving with the same velocity, was carried out in order to compare with the chemical boundary layer solution. The results are shown in Figs. 4, 5 and 6.

VI. RÉSUMÉ

Experiments (2) and the success of the existing theories on laminar diffusion flames have clearly shown that, in those cases where a stable laminar diffusion flame has been obtained, the Burke-Schumann assumption (infinitely fast reaction rate) applies. However, the Burke-Schumann solution is independent of chemical kinetics, and does not give any criterion either for flame extinction or for the validity of the solution.

The fact that in this solution the flame thickness is zero suggests that in practical cases the reaction zone must be of negligible thickness, making it possible to obtain a solution of the boundary layer type including the effects of chemical kinetics.

At each side of the extremely thin reaction zone, chemical reaction effects are neglected as compared with convection, conduction, and diffusion effects. The reaction zone reduces to a flame front of negligible thickness, which acts as a sink for the reactants and as a source for the heat and products evolved in the chemical reaction. The location of the flame front, rate of burning, and temperature and concentration distributions in the exterior of the reaction zone are determined by using the Burke-Schumann assumption.

In order to analzye the structure of the burning zone we may neglect in it convection effects as compared with conduction, diffusion and chemical reaction effects. The equations

governing this chemical boundary layer are ordinary differential equations with boundary conditions determined by the Burke-Schumann solution. Temperatures there are close to the adiabatic flame temperature, and then an overall kinetic scheme applies.

The criteria for extinction of the flame and for the validity of Burke-Schumann assumption approximately coincide, and may be obtained by solving, once the Burke-Schumann solution is known, the chemical boundary layer equations. This solution also provides the temperature and concentration distributions in the reaction zone.

If our main purpose is the evaluation of the chemical kinetic effects in diffusion flames an approximate solution of the Burke-Schumann mixing problem will be sufficient. This we may obtain easily for large Reynolds numbers by using well known boundary layer approximations.

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APPENDIX A

In this appendix an integral method for the approximate solution of equation [31] is presented. We will use the same approximations as those used in obtaining [37] from [36]. We will consider the more general mass production rate expression given by [7]. Then, if relations [35] are taken into account, by taking [7] into [31], we obtain

$$\frac{d^2\theta}{dy_1^2} = -\frac{\nu^b T^{*a+b-1}}{D_0 t_c}\cdot\chi\cdot\left|1-\theta+\frac{\nu}{K_{20}}\cdot\frac{y_2}{\delta_m}\right|^a\cdot\left|1-\theta-\left(\frac{1}{T_f^*}-\frac{\nu}{K_3}\right)\frac{y_1}{\delta_m}\right|^b. \qquad [A.1]$$

Where

$$\chi = \frac{g(T_c,p)}{g(T_f,p_0)}\exp\left\{\frac{-E}{RT_f}\frac{T_f-T_c}{T_c}\right\}$$

and

$$t_c^{-1}=g(T_f,p_0)\exp\{-E/RT_f\}. \qquad [A.2]$$

Here, however, we will not choose $T_c(x)$ as the temperature at $y_1=0$, but as the temperature at a point that we will determine later on.

By introducing the variables

$$\beta=\left|4\nu^b\frac{\delta_m^2}{D_0 t_c}\chi\right|^{-\frac{1}{a+b+1}} T_f^*\left\{1-\theta+\left(\frac{\nu}{K_{20}}-\frac{1}{2T_f^*}\right)\frac{y_1}{\delta_m}\right\} \qquad [A.3]$$

$$z=\frac{1}{2}\left|4\nu^b\frac{\delta_m^2}{D_0 t_c}\chi\right|^{\frac{1}{a+b+1}}\frac{y_1}{\delta_m} \qquad [A.4]$$

equation [A.1] transforms to

$$\frac{d^2\beta}{dz^2}=-(\beta-z)^a(\beta+z)^b. \qquad [A.5]$$

That must be solved with the boundary conditions

$$\beta-z\to 0 \qquad \text{for} \qquad z\to+\infty.$$

In order to solve equation [A.5] in an approximate way, we will use the following integral method.

If z_1 is the point where β'' reaches its maximum value, the right hand side of equation [A.5] may be written in the form

$$(\beta_1-z_1)^a(\beta_1+z_1)^b e^{-h(z)}.$$

Where

$$\beta_1=\beta(z_1) \qquad \text{and} \qquad h(z)=k^2(z-z_1)^2+\cdots.$$

From [A.10] we deduce

$$z_1 = \frac{b-a}{b+a}\,\beta_1, \qquad \beta_1 + z_1 = \frac{2b}{a+b}\,\beta_1, \qquad \beta_1 - z_1 = \frac{2a}{a+b}\,\beta_1. \qquad [A.12]$$

Then from [A.9], [A.11] and [A.12] we get the relation

$$\left(\frac{2a}{a+b}\right)^a \left(\frac{2b}{a+b}\right)^b \frac{a+b}{\beta_1}\,\beta_1^{a+b} - \frac{(a+b)^3}{4ab}\,\frac{1}{\beta_1^2} = \frac{\pi}{2}\left(\frac{2a}{a+b}\right)^{2a}\left(\frac{2b}{a+b}\right)^{2b}\beta_1^{2(a+b)} \qquad [A.13]$$

that has the solution, if $1/(a+b+c)=s$,

$$\beta_1 = \frac{a+b}{2}\left[\frac{2}{\pi a^a b^b}\left(\sqrt{1+\frac{\pi(a+b)}{2ab}}-1\right)\right]^s. \qquad [A.14]$$

Now z_1 and k may be determined in terms of β_1 by means of the relations

$$z_1 = \frac{b-a}{b+a}\,\beta_1 \qquad \text{and} \qquad k = \sqrt{\frac{\pi}{2}}\left(\frac{2a}{a+b}\right)^a\left(\frac{2b}{a+b}\right)^b \beta_1^{a+b}. \qquad [A.15]$$

As an approximate solution of equation [A.1] we may use either the function

$$\beta(z) = \beta_1 + (z-z_1)\mathrm{erf}\,k(z-z_1) + (\sqrt{\pi}\,k)^{-1}\{1-\exp(-k^2(z-z_1)^2)\} \qquad [A.16]$$

obtained by integrating equation [A.6], or the more approximate, but also more difficult to evaluate, function $\beta(z)$ solution of the algebraic equation [A.8]. In both cases the parameters β_1, z_1 and k are as given by [A.14] and [A.15].

In order to compare the above approximate solutions of equation [A.5] with the exact numerical solution, we consider the particular case $a=1$, $b=1$. Then

$$\beta_1 = 0.87, \qquad z_1 = 0, \qquad k = 0.67 \qquad [A.17]$$

and

$$\beta(z) = 0.87 + z\,\mathrm{erf}\,0.67z + 0.84[1-\exp-(0.67z)^2] \qquad [A.18]$$

$$\beta(z) = [z^2 + 0.76\exp-(0.67z)^2]^{1/2}. \qquad [A.19]$$

The approximate solution $\beta(z)$ has been plotted with a dashed line in Fig. 2 to compare with the exact solution drawn with a solid line.

Going back to the general case in which a and b are not necessarily one, let us choose the temperature at the point z_1 as the temperature used in approximating equation [31].

Then from relation [A.3] by making $z=z_1$, we get

$$(1-\theta_c)\left[4+\sqrt{\frac{\partial^2_{zz}(x)}{D_{zz}t}\,\chi(x,\theta_c)}\right] = \frac{\beta_1}{T_f^*}\left[1+\left(\frac{2\sqrt{T_f^*}}{K_{zc}}-1\right)\frac{b-a}{b+a}\right]. \qquad [A.20]$$

This is an algebraic equation for θ_c.

Again a first approximation to the solution is obtained by making $\theta_c = 1$ when evaluating $\chi(x, \theta_c)$. Then relation [A.20] transforms to

$$\theta_c = 1 - \frac{\beta_1}{A_0^s} \qquad [A.21]$$

where

$$A_0 = 4 \nu^b \frac{\delta_m^2(x)}{D_0 t_c} \chi(x, 1) \left\{ T_f^* \middle/ \left| 1 - \left(\frac{2\nu T_f^*}{K_{20}} - 1 \right) \frac{b - a}{b + a} \right| \right\}^{1/s}$$

and

$$\chi(x, 1) = 1 \qquad \text{if} \qquad p = p_0.$$

A second approximation, similar to 45, may be obtained for θ_c without major difficulties.

APPENDIX B

In order to approximately solve the Blassius equation

$$f''' + f f'' = 0 \qquad [B.1]$$

with the boundary conditions

$$f'(\infty) = 1, \qquad f'(-\infty) = \lambda, \qquad f(o) = 0,$$

following Meksyn (27) let us write equation [B.1] in the form

$$\frac{f'''}{f''} = -f = -a_1 \eta - \frac{a_2}{2} \eta^2 + \frac{a_1 a_2}{24} \eta^4 + \cdots \qquad [B.2]$$

where $a_1 = f'(o)$ and $a_2 = f''(o)$ are assumed to be known.

Then by integrating [B.2] twice we get

$$f' - a_1 = a_2 \int_0^\eta \exp \left\{ - \left(\frac{a_1}{2} \eta^2 + \frac{a_2}{6} \eta^3 + \cdots \right) \right\} d\eta. \qquad [B.3]$$

As the shear stress decreases very rapidly with increasing values of $|\eta|$, we may expect that most of the contribution to the integral [B.3] comes from those low values of $|\eta|$, for which f can be well approximated using only the first terms in the power series expansion [B.2].

If we write

$$\frac{a_1}{2} \eta^2 + \frac{a_2}{6} \eta^3 + \cdots = \tau$$

then

$$\eta = -\left|\sqrt{\frac{2\tau}{a_1}}\left(1 + \frac{a_2}{6a_1}\right|\sqrt{\frac{2\tau}{a_1}} + \cdots\right) \quad \text{for} \quad \eta < 0$$

$$\eta = \left|\sqrt{\frac{2\tau}{a_1}}\left(1 - \frac{a_2}{6a_1}\right|\sqrt{\frac{2\tau}{a_1}} + \cdots\right) \quad \text{for} \quad \eta > 0$$

[B.4]

Then the integral [B.3] may be evaluated and we obtain

$$f' = a_1 + \frac{a_2}{|2a_1}\left[|\pi \operatorname{erf}|\tau - \frac{|2\,a_2}{3a_1^{3/2}}(1 - e^{-\tau}) + \cdots\right], \quad \eta > 0$$

$$f' = a_1 - \frac{a_2}{|2a_1}\left[|\pi \operatorname{erf}|\tau + \frac{|2\,a_2}{3a_1^{3/2}}(1 - e^{-\tau}) + \cdots\right], \quad \eta < 0$$

[B.5]

If we now make $\tau \to \pm \infty$, we obtain

$$1 = a_1 + \frac{a_2}{|a_1}\left|\sqrt{\frac{\pi}{2}}\left[1 - \frac{a_2}{3a_1^{3/2}}\right|\sqrt{\frac{2}{\pi}} + \cdots\right]$$

$$\lambda = a_1 - \frac{a_2}{|a_1}\left|\sqrt{\frac{\pi}{2}}\left[1 + \frac{a_2}{3a_1^{3/2}}\right|\sqrt{\frac{2}{\pi}} + \cdots\right]$$

[B.6]

The series in [B.6] may be expected to converge very rapidly. Keeping only the first two terms of the series expansions appearing within brackets in [B.6], we get

$$1 - \lambda = \left|\sqrt{\frac{2\pi}{a_1}}\,a_2\right.$$

and

$$a_1 = \frac{1 + \lambda}{2}\left[1 - \frac{1}{2}\left|1 + \frac{8}{3\pi}\left(\frac{1-\lambda}{1+\lambda}\right)^2\right|\right]$$

[B.7]

that may be approximated with less than 4% error by

$$a_1 = \frac{1+\lambda}{2}\left[1 - \frac{2}{3\pi}\left(\frac{1-\lambda}{1+\lambda}\right)^2\right]$$

$$a_2 = \frac{1-\lambda}{|2\pi}\left|\frac{1+\lambda}{2}\left[1 - \frac{1}{3\pi}\left(\frac{1-\lambda}{1+\lambda}\right)^2\right]\right|$$

[B.8]

Now by means of relations [B.8] the solution [B.5] may be written up to the second approximation. A first approximation is

$$f'(o) = \frac{1+\lambda}{2}, \qquad f''(o) = \frac{1+\lambda}{2}\left|\frac{1+\lambda}{\pi}\right.$$

$$f = \frac{1+\lambda}{2} + \frac{1+\lambda}{2}\operatorname{erf}\left|\frac{1+\lambda}{2}\,\eta\right.$$

[B.9]

APPENDIX C

Low Speed Source Flow.

The laminar diffusion flame produced when a point source of fuel is immersed in an oxidizer stream has been qualitatively discussed by Penner (28).

Let the density and temperature of the fuel leaving the source be equal to the density and temperature of the oxidizer stream. If $\dot{M}$ is the mass rate of supply of fuel due to the source, the velocity distribution is given by

$$\vec{v} = \nabla \left(U_\infty x_3 + \frac{\dot{M}}{4 \pi \rho_0 r_1} \right) \tag{C.1}$$

where $r_1 = \sqrt{x_1^2 + x_2^2 + x_3^2}$ and the x_3 axis is in the free, oxidizer, stream direction. The source is located at the origin and U_∞ is the free stream velocity.

The stream surface that separates fuel and oxidizer is easy to calculate, and that has been done elsewhere. In particular, the radius of curvature at the stagnation point is

$$R_0 = \left(\frac{\dot{M}}{4 \pi \rho_0 U_\infty} \right)^{1/2}. \tag{C.2}$$

Then Λ_0 at the stagnation point may be evaluated by using relations [44] and [63]. We obtain

$$\Lambda_0 \sim \frac{\dot{M}}{\rho_0} \frac{1}{U_\infty^{3/2} l_r} . \tag{C.3}$$

Therefore the criterion for either the validity of the Burke-Schumann assumption or for extinction is practically independent of the transport properties. They enter only through the values of Pr and Sc.

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